The Nuclear Reaction Code McGNASH

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We are developing a modern version of the GNASH nuclear reaction code [1], which has been used successfully over the years to compute neutron-, proton-, and photon-induced reactions cross sections on a variety of nuclei targets, and for incident particle energies from tens of keV up to 150–200 MeV. This code has been instrumental in producing numerous nuclear data evaluation files for various ENDF (Evaluated Nuclear Data Files) libraries around the world, and in particular the ENDF/B-VI and pre-ENDF/B-VII libraries in the U.S. More recently, GNASH was used extensively for the creation of the LA150 library [2], containing data on neutron- and proton-induced reactions up to 150 MeV incident energy.

Written in old FORTRAN, the GNASH code was born in the early seventies and was continuously improved since then to incorporate new physics models. However, in doing so, the structure of the code has become very complicated and somewhat cumbersome to upgrade or even simply maintain. The advent of the modern FORTRAN 90/95 scientific language has opened the path toward modern and higher-level programming techniques that can be implemented efficiently to create a modern and more powerful version of the GNASH code.

This new code is called McGNASH and is being written in FORTRAN 95. It uses the concept of modular programming extensively. In fact, the McGNASH code is really a collection of such FORTRAN modules, each dealing with a specific (and often independent) part of the nuclear reaction sequence calculation. These modules are always written with the ideas of robustness and capacity to evolve in mind. The coding in McGNASH is strongly influenced by the notion of object-oriented programming, though it does not make use of some specific characteristics of this type of programming.

McGNASH is also being written with the user in mind. While a default GNASH input can be cumbersome to read or/and build for the nonexpert, a McGNASH input has been reduced to a very simple and compact form, which can be easily tuned to any user's needs. We hope that this move will encourage the broad use of McGNASH outside its developer base community. Of course, simplicity and compactness come at a price. The same parameters appearing explicitly in a GNASH input are now "hidden" as default parameters in a McGNASH calculation. For simple and default calculations (or for producing large amounts of data over a large portion of the nuclear landscape), this last solution is certainly the best. However, in case the physics at hand is only poorly known, a default calculation might easily lead to relatively wrong answers, which only an expert-eye can detect. Hence, a word of caution may be worthwhile here.

In order to get default calculations running for the most common nuclear reaction data needs, it is necessary to provide the code with default input data (e.g., discrete level schemes, optical model parameters, etc.). To do so, we have chosen to link the RIPL-2 database [3] directly to McGNASH, hence providing default data for many nuclei and nuclear reactions.

For evaluation work, performing a nuclear reaction calculation is just not enough. The extraction and formatting of the pertinent results in a ENDF-type file is required. To achieve this task, GNASH uses an auxiliary code called GSCAN, which needs to be run independently of GNASH. With McGNASH, this feature will be automatically available.

The basic physics models that constitute the backbone of the GNASH code are also present in McGNASH. A neutron- or proton-induced reaction on a heavy target leads to the formation of a compound nucleus in statistical equilibrium, which then decays by emitting gamma-rays, neutron or light-charged particles, until a stable ground- or

isomeric-state is reached. The assumption of a compound nucleus in equilibrium breaks down at low- (very few open channels) and high- (emission of pre-equilibrium high energy particles) incident energies. Both the coding and the physics models used to calculate the needed corrections to the statistical picture represent a great improvement in McGNASH with respect to GNASH.

At low-incident energies, the so-called width fluctuation correction factors are calculated within three models: HRTW, Moldauer, and exact Gaussian Orthogonal Ensemble (GOE). The two first models represent only approximations to the exact GOE calculation, which however takes significantly longer to compute. Figure 1 provides an overview of the domain of validity of both HRTW's and Moldauer's methods.
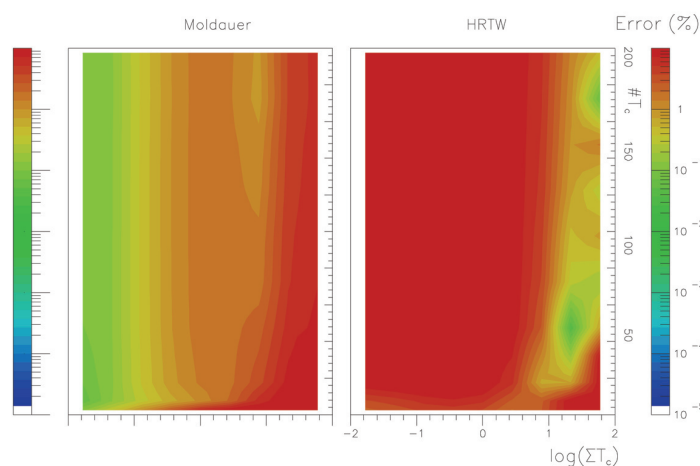
At high-incident energies, the DDHMS Monte Carlo code by Chadwick is used within McGNASH, implementing the Hybrid Monte Carlo model by Blann and Chadwick [4]. This model has several important advantages over the exciton model, implemented in the GNASH code. In particular, the DDHMS approach can be used to predict the residual spin distribution of the excited nucleus after the emission of pre-equilibrium nucleons. This distribution can differ significantly from the Hauser-Feshbach compound nucleus spin distribution, depending on the number and energy of the pre-equilibrium ejectiles. In applications particularly sensitive to the conservation of angular momentum (e.g., branching ratios to spin isomers, or precise determination of γ-ray lines in a gamma-cascade), it is important to calculate this residual spin distribution accurately. An example of such calculated residual spins distributions after pre-equilibrium emission is shown in Fig. 2 for protons (160 MeV) on ^{90}Zr.
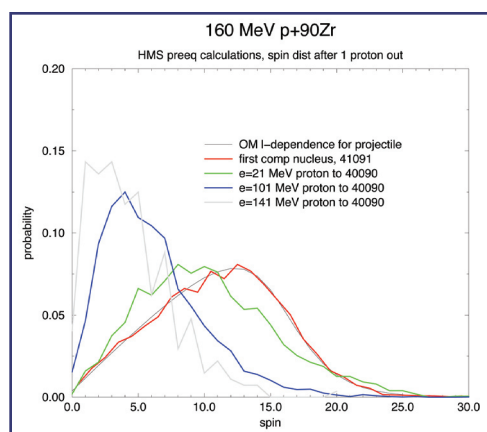

A first version of McGNASH is expected to be released by the end of 2005.

[1] P.G. Young, E.D. Arthur, and M.B. Chadwick, Proc. Workshop on *Nuclear Reaction Data and Nuclear Reactors*, ICTP Trieste, Italy, April 15–May 17, 1996 (World Sci. Publ. Co., Singapore, 1998), pp. 227–404.
[2] M.B. Chadwick, et al., *Nucl. Sci. Eng.* **131**, 293 (1999).
[3] "*Reference Input Parameter Library RIPL-2*," http://www-nds.iaea.org.
[4] M. Blann and M.B. Chadwick, *Phys. Rev. C* **57**, 233 (1998).

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